Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots

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NEMO 3-D has been developed for the simulation of electronic structure in self-assembled InGaAs quantum dots on GaAs substrates. Typical self-assembled quantum dots in that material system contain about 0.5 to 1 million atoms. Effects of strain by the surrounding GaAs buffer modify the electronic structure inside the quantum dot significantly and a large GaAs buffer must be included in the strain and electronic structure. However, to reduce computational expenses it is desirable to keep the GaAs buffer as small as possible. The simulations presented in this paper analyze the local band structure in the system as well as the dependence of the confined hole and electron states in ensembles of alloyed InGaAs quantum dots on the total strain of the system and the GaAs buffer size.

The local strain in the 3-D system modifies bond lengths and angles for individual atoms in a unit cell. Local band structure can be computed with a periodic repetition of such a unit cell. InGaAs alloys maintain a bi-modal distribution of InAs and GaAs-like bond length resulting in a bi-modal distribution of local band edges. Figures 1a and 1b show a scatter plot of local conduction band edges along a line laterally through a 30nm diameter, 5nm high dome shaped $In_{0.6}Ga_{0.4}As$ quantum dot for two different buffer sizes. The bi-modal distributions of InAs and GaAs-like band edges are evident inside the quantum dot. The GaAs-like bonds are compressed by the surrounding InAs resulting in local band edges that are higher than the surrounding GaAs. The InAs-like bonds are compressed by the overall surrounding GaAs resulting in a local band edge raised from the unstrained value. The 4nm and 12nm buffer layer simulations show significantly different scatter of local band edges in the quantum dots. 2^{nd} degree polynomial fits in the spatial regions of the buffer and central quantum dot region are shown in Figure 1a-b) as well for InAs and GaAs-like bonds. The interface regions are left out the fits because of the distributed interface of the InGaAs dome shaped dot. The dashed lines in the quantum dots show the average local band structure including both InAs and GaAs-like bonds. Figure 1c compares the average local potentials for the 4nm and 12nm buffer size. The effects of the different buffer size are clearly evident.

We have previously analyzed the statistical distribution of electron and hole ground state energies in InGaAs quantum dots. Here we analyze the effects of the finite GaAs buffer sizes on the statistical energy distribution and their dependence on the local strain energy. The electron and hole ground states are computed in two ensembles of 200 random alloy InGaAs quantum dots for a 4nm and 8nm surrounding GaAs buffer assuming open strain boundary conditions. The ground state energies are graphed in a scatter plot against the total strain energy in the system in Figure 1a-d). Several observations can be made: 1) the absolute average energies vary with the buffer size (band gap increases with increasing buffer size), 2) the standard deviation induced by random disorder decreases with increasing buffer size, 3) the dependence on the total strain in the system is reduced for increasing buffer size. Some of these characteristics can be immediately shown to be dependent on the local band structure in the quantum dot and the surrounding buffer size. The 4nm buffer clearly is not enough to properly model the effect of the surrounding GaAs buffer.

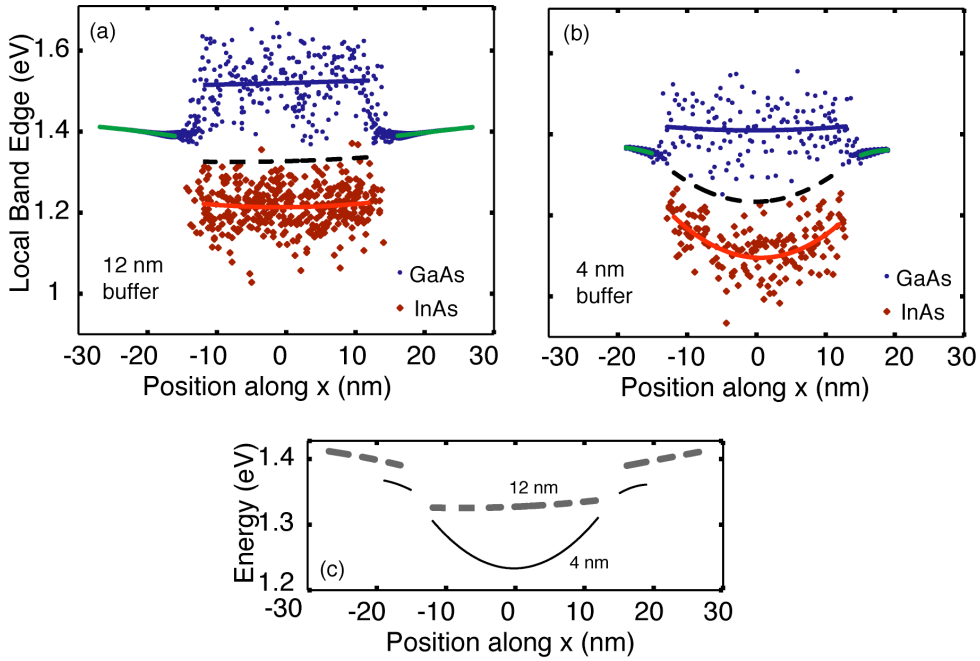

Figure 1: (a-b) Local band edge along a line laterally through an InGaAs/GaAs quantum dot system for two GaAs buffer sizes. Bi-modal distribution of InAs and GaAs bond lengths in InGaAs leads to a bi-modal distribution of local band edge energies computed in a single primitive cell. Solid lines are 2nd order polynomial fits to the scatter. Dashed line is a fit to the overall band edge inside the quantum dot. (c) Average confining potentials from (a) and (b). Small buffer size imposes a significantly more bent potential profile inside the quantum dot.

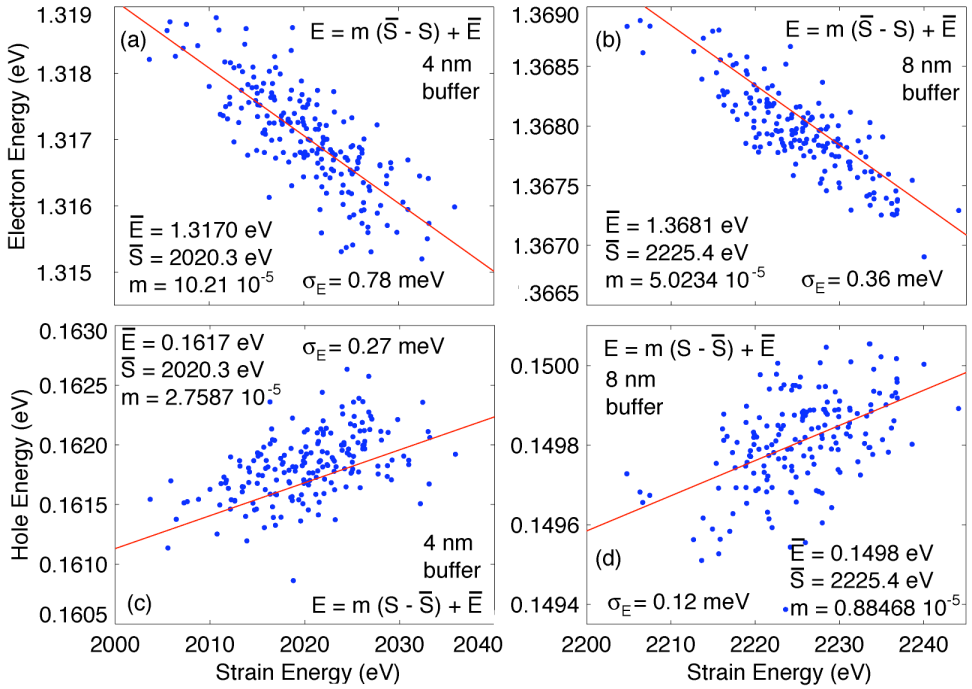

Figure 2: (a-d) 200 statistical samples for each buffer size of electron and hole eigen energies with their corresponding in InGaAs quantum dots plotted against the total strain energies. Electron energies are decreasing with increasing strain while hole energies are increasing with increasing strain. The solid lines represent linear regression fits and are referenced to the average strain and average electron/hole energy. Increasing the buffer size from 4nm to 8nm reduces the sensitivity of the eigen energies to strain (reduced slope factor m) and reduces the statistical noise in the statistical variation in the eigen energies (reduced σ_E).